Emergence of robust gaps in 2D antiferromagnets via additional spin-1/2 probes

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We study the capacity of antiferromagnetic lattices of varying geometries to entangle two additional spin-1/2 probes. Analytical modeling of the Quantum Monte Carlo data shows the appearance of a robust gap, allowing a description of entanglement in terms of probe-only states, even in cases where the coupling to the probes is larger than the gap of the spin lattice and cannot be treated perturbatively. We find a considerable enhancement of the temperature at which probe entanglement disappears, as we vary the geometry of the bus and the coupling to the probes.

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Solid state systems have been exploited to integrate quantum information (QI) tasks and accomplish quantum computation in a single processing core, but many questions regarding their robustness against temperature and decoherence remain open. Among the requirements to achieve quantum computation, the ability to generate rapid elementary gates between well-characterized qubits is central [1]. In view of the technical difficulties of switching on direct interactions between qubits, various proposals have been put forward to use a quantum sub-system, usually denominated as *bus,* to mediate the fundamental universal gates. It can be realized, for instance, by the phononic mode of cold ions, in the famous ion-trap quantum computer [2], or by the magnetic degrees of freedom of a quantum spin chain (see [3] and references therein). A considerable body of work has been devoted to chains of spins experiencing nearest-neighbor interactions, since they can be used as models for universal quantum computation, meeting the aforementioned requirements [4]. Spin chains have been shown to be extremely versatile; for instance, they allow the reliable transfer of the state of a single qubit [5], and their ground-states are able to mediate an effective long-distance interaction ultimately entangling distant spin probes — the so-called long-distance entanglement (LDE) [6, 7].

Promising advances in the engineering of atomic structures and optical lattices, where finite spin systems are effectively realized in the laboratory, encourage the consideration of more general possibilities. We consider antiferromagnetic (AF) spin systems, ranging from 1D chains to square lattices, and demonstrate the opening of robust gaps via local interactions with two additional spin-1/2 particles. Robust gaps implies negligible thermal occupation of excited bus states in the entire range of temperatures in which the probes are entangled; this allows for QI capabilities (*e.g.* LDE) at higher temperatures than previously considered possible.

Models of spins — We start by making precise the notion of "robust gap"; by this we mean that the bus plus probes system has a low energy manifold isomorphic to the probe space, well separated in energy from the remaining energy spectrum (see Figures 1 and 2). Should this be so, and for the case of rotational invariant cou-

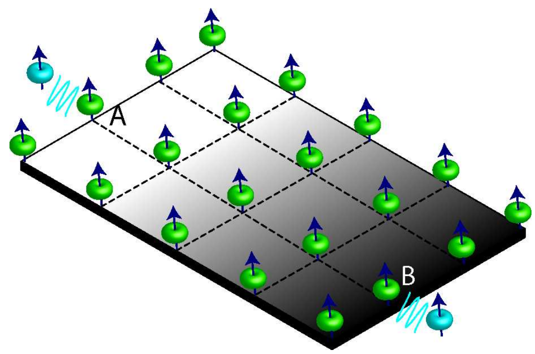

Figure 1: The probes (blue) interact locally with the lattice through sites A and B. Will the bus create an effective interaction capable of entangling the probes at finite temperature?

plings, symmetry alone allows for an analytical description of the temperature dependence of the entanglement between probes. Surprisingly, we found that in all the systems we studied by means of Quantum Monte Carlo (QMC) simulations, entanglement follows this description very accurately. This shows that, even in systems where the bus has a very small gap (approaching zero in the thermodynamic limit), the actual coupling to the probes can ensure the emergence of a robust gap, an ideal situation for quantum computation.

We consider two qubit probes that interact locally with a generic finite spin lattice (the bus). Setting $\hbar = 1$, the Hamiltonian of the full system (bus + probes) reads,

$$H = H_{bus} + \alpha J \left(\tau_a \cdot S_A + \tau_b \cdot S_B\right), \qquad (1)$$

where H_{bus} is the Hamiltonian of the bus, αJ is the coupling strength between the probe qubits and the lattice, and J a characteristic energy scale of the bus. Eq. (1) describes an isotropic interaction between the probes - with Pauli operators, $\vec{\tau}_{A(B)}$ - and the bus spins at specific lattice sites ($\vec{S}_{A(B)}$; $A, B \in \mathcal{L}$). We speak about LDE at temperature $k_B T = 1/\beta$, whenever the partial state of the probes is entangled for distances of the order of the system size, $d_{AB} \sim O(L)$. Genuine quantum correlations among qubits living in the bulk system usually decay rapidly [8], and, only recently, one-dimensional

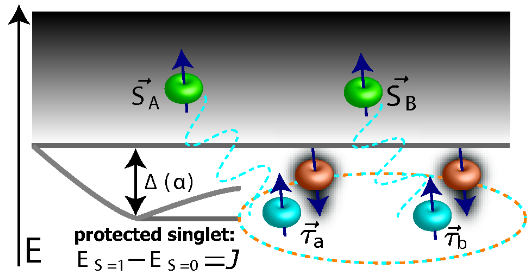

Figure 2: Schematic of the opening of a robust gap ($\Delta(\alpha) \gg k_B T$) by two spin-1/2 probes that couple locally to the many-body system (bus) with arbitrary strength αJ. This is observed in all the AF lattices considered in this article. If the singlet is localized near the additional probes, they will be highly entangled even at large distances - the so-called LDE. The singlet has a protection gap (triplet-singlet energy separation, $\mathcal{J}$) which is enhanced with the dimensionality of the bus.

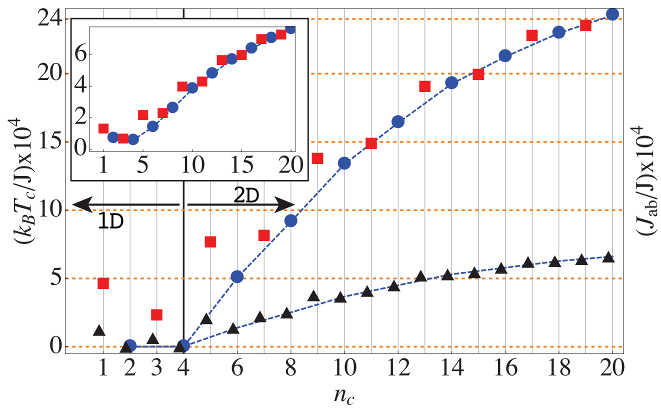

Figure 3: Black triangles: effective coupling, J_{ab}, at a distance $l = 20$, as a function of n_c, number of transverse chains ($k_B T = 2 \times 10^{-3} J$); blue dots and red squares: critical temperature above which LDE vanishes; inset: canonical coupling (*i.e.* the probes singlet protection gap of Fig. 2), in the same units used to represent J_{ab}. The error bars from QMC cannot be seen as they are typically below 1%; $\alpha = 0.05$ in all plots.

spin systems were found to support robust LDE [6, 7], as opposed to gapless bosonic systems [9].

We focus on $SU(2)$ symmetric Heisenberg interactions, which not only allow universal quantum computation [3], but are also commonly realized in nature (*e.g.* in the parent compounds of copper-oxide high-temperature superconductors, such as the undoped insulator La_2CuO_4 [10]; in electronically coupled quasi- 1D chains such as $CuGeO_3$ [11]; in the Mott insulating one-dimensional perovskite, $KCuF_3$ [12]; in linear chains of ~ 10 manganese atoms in engineered structures [13]).

The partial state ρ_{ab} is completely fixed by symmetry and depends on a single physical parameter driving the bus capacity to entangle the probes,

$$\rho_{ab} = \mathcal{Z}_{ab}^{-1} \exp\left(-\beta J_{ab} \tau_a \cdot \tau_b\right). \quad (2)$$

The effective coupling changes with temperature, $J_{ab} = J_{ab}(\beta)$, since tracing out the degrees of freedom in $\mathcal{L}$ introduces mixedness. A QMC calculation of the correlation between probes allows easy extraction of $J_{ab}(\beta)$. As it stands, Eq. (2) would mark no real advance, if not for the fact that symmetry allows a complete specification of the temperature dependence of the effective coupling $J_{ab} = J_{ab}(\beta)$, provided the condition of a robust gap is verified; J_{ab} can be expressed as function of three temperature independent parameters ($\mathcal{J}$, Φ and η) in the entire parameter region where the probe entanglement is not too small:

$$J_{ab}(\beta) = \frac{1}{4\beta} \ln\left[\frac{3(\Phi - \eta) + (4 - 3\Phi - \eta)e^{\beta\mathcal{J}}}{4 - \Phi + \eta + (\Phi + \eta/3)e^{\beta\mathcal{J}}}\right]. \quad (3)$$

The canonical coupling $\mathcal{J}$ is the gap between the lowest singlet and triplet (the protection gap), and sets the temperature scale for the disappearance of entanglement. The canonical corrections, Φ and η, determine the amount of entanglement at zero temperature (see Appendix). Although these parameters cannot be analytically computed in general, they are well-approximated by their values in perturbation theory for α sufficiently small. For weak coupling, it turns out that $\eta \ll \Phi$, since the first non-zero contribution to η is of order α^4, whereas $\Phi \sim \mathcal{O}(\alpha^2)$. The formula (3) is exact and will be valid whenever the bus–probe system has a robust gap.

Numerical results: Effective interaction enhancement in 2D — We now present the main results from the QMC simulations on a family of AF lattices and compare the results with our theoretical prediction [Eq. (3)]. Our systems consist of 2-dimensional (2D) finite lattice $\mathcal{L}$, with $N = l \times n_c$ spins-1/2 and two extra probes, where l is the number of longitudinal sites and n_c stands for the number of coupled chains, varying from $n_c = 1$ to $n_c = l$. The Hamiltonian of the lattice is $H_0 = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$, with $J > 0$. The qubit probes interact with the spins at the boundary of the most central chain (see Fig. 1) through an isotropic interaction [Eq. (1)]. We expect a significant change in the LDE from the common one-dimensional scenario [6], as the physics of a 2D bus is very distinct. In particular, the 2-leg ladder chain has an Haldane gap which should play against a large J_{ab} since very *massive excitations*, $\Delta \simeq 0.504J$, make the correlations die particularly fast [14].

We briefly present the results for small probe-bulk coupling, $\alpha = 0.05$, before venturing away from perturbation theory. The results of Fig. 3 and Fig. 4 show a clear enhancement of the ability of the antiferromagnet to generate long-range effective interactions among distant probes as one reaches the square-lattice. Also, a wiggly behavior up to $n_c = 4$ is evident (the large Haldane

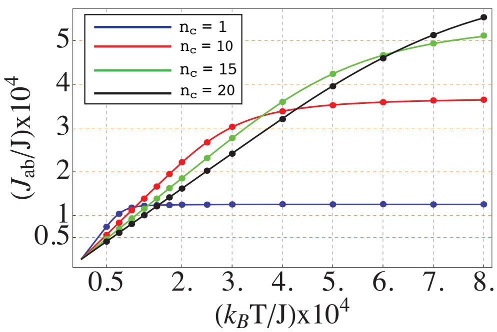

Figure 4: The points in the plot show J_{ab} as function of the temperature from the QMC simulations for $\alpha = 0.05$. The lines stand for the fit with the expression given in Eq. (3). All curves saturate for high-temperatures [Eq. (4)] and therefore entanglement vanishes much before our method becomes inaccurate. The agreement between the QMC data is excellent resulting in a average deviation of $\sim 0.1 - 1\%$ depending on the lattice.

gap for $n_c = 2$ and 4 implies a fast decay of correlations within the bulk spins leading to a negligible effective coupling). Fig. 3 shows a curious transition for $n_c > 4$: the increase of the protection gap $\mathcal{J}$ (and also J_{ab}) becomes smooth and the Haldane finite-size gap, very strong for $n_c = \{2, 4\}$, gets suppressed — the $2D$ physics is reached monotonously as the bus gap disappears.

We expect the ground state of $2D$ antiferromagnets to reduce substantially the LDE due to the symmetry breaking at $T = 0$, for large lattices; the finite staggered magnetization should reduce the amount of genuine quantum correlations shared by the probes. This is borne out by the results of the QMC simulations, shown in Fig. 4, where J_{ab} is found to decrease at low temperatures, when the number of chains increase. Nevertheless, at higher temperatures, the opposite occurs, J_{ab} increases with n_c; this reflects the increase of the protection gap, $\mathcal{J}$. Having shown the QMC results for 20 spin lattices, we now compare them with Eq. (3) for several temperatures: Fig. 4 shows a perfect fit to the QMC data. For sake of clarity, we have presented the agreement just for 4 lattices although all them show the same degree of accuracy. The observed linear dependence of J_{ab} with the temperature for $T \to 0$ is easily understood: a zero temperature (finite) entanglement below the maximum value of 1 requires $J_{ab}/T \to$ constant (see Fig. 5). This constant can be derived from Eq. (3), yielding, $4\beta J_{ab} \underset{\beta\to\infty}{\longrightarrow} \ln\left[(4 - 3\Phi - \eta)/(\Phi + \eta/3)\right]$; thus, the *canonical corrections* (Φ and η) determine the low-temperature physics of the probes. For high-temperatures the effective coupling satures (see Fig. 4) to a constant value, $\mathcal{J}(1-\Phi)$, when η is negligible (*i.e.* not far away from the perturbation limit, see Eq. (6) and comments therein), suffering a slightly increase otherwise,

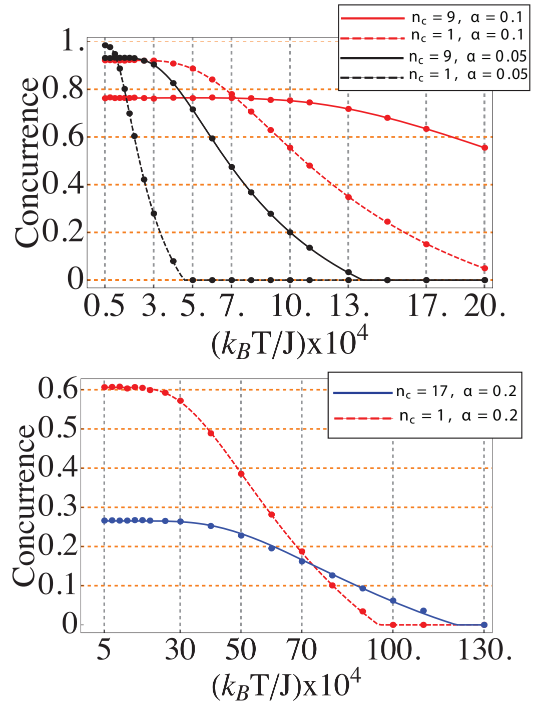

Figure 5: Concurrence, an entanglement monotone for qubits, as function of temperature for representive lattices and different couplings. Lattices supporting more entanglement at strictly $T = 0$ have worse performance at higher temperatures.

$$J_{ab}(T) = \frac{\mathcal{J}\,(1-\Phi)}{4\,(1-\eta)\,(1+\eta/3)} + \frac{k_B T}{4}\ln\left(\frac{1-\eta}{1+\eta/3}\right) + O\left(\frac{\mathcal{J}^2\Phi}{k_B T}\right). \tag{4}$$

Figures 3 and 4 deal with relatively small probe-bus coupling, but the results presented so far are more general. For instance, choosing a sufficiently large α to strongly suppress the zero temperature entanglement, due to partial frustration among the neighborhood of the bulk spins connected with the probes, we again find an excellent agreement with Eq. (3); the measured concurrence is perfectly fitted with an expression derived from Eq. (3) (see Fig. 5). This clearly shows that in all our measured systems, the condition of a robust gap is verified. This is surprising, particularly in the case of the (finite) square lattice, which has a gap much smaller than αJ; one would not expect, in this situation, the appearance of a well protected singlet. The emergence of the robust gap has to be *attributed to the coupling of the probes*: the lowest singlet and triplet are pulled down from the rest of the spectrum, allowing a complete description of entanglement only in terms of these two energy levels. On the other hand, whereas this stronger coupling to the bus reduces the zero temperature entanglement, it also allows a larger split between the singlet and triplet, leading to entangled probes at much higher

temperatures. Typically, exchange interactions in antiferromagnets can be of the order of 0.1 eV, resulting in an effective coupling of the order of 0.3 meV for the square lattice ($l = 20$) at temperature $\sim 12\,\mathrm{K}$ and $\alpha = 0.2$. This is to be compared with the value of $0.01 - 0.1$ meV achievable in quantum dot spins [15] (see comment [17]). Regarding LDE (see also Fig. 5) we see that the critical temperature (above which the correlations shared by the probes are completely classical) can be increased by a factor of 20 from weakly coupled spin chain ($\alpha = 0.05$) to an intermediate coupled ($\alpha = 0.2$) square lattice, entanglement surviving up to $k_B T \simeq 1.2 \times 10^{-2} J$.

Conclusions — We observed an enhancement of LDE by varying the geometry of the magnetic spin systems serving as a quantum bus. The analysis based on the canonical transformation formalism agrees very well with the results from QMC simulations, demonstrating the emergence of robust gaps in AF lattices via a coupling of intermediate strength with external probes. We raise the possibility of entangling distant spin probes at temperatures as high as $T \simeq 1.2 \times 10^{-2} J/k_B$, where J is the nearest neighbor exchange constant of the bus. We hope this work stimulates research in the area of "all-in-one" solid-state based quantum communication and computation.

Appendix: Analytic treatment and the canonical parameters — We take the bus to be a spin 1/2 spin system with rotationally invariant couplings and a non degenerate singlet ground state $|\phi_0\rangle$; the probes couple to the bus also through isotropic couplings, Eq.(1). If adiabatic continuity holds [16], we have a one-to-one map of the eigenstates of the full Hamiltonian to those of $\alpha = 0$ (uncoupled probes); this map defines a canonical transformation, $|\phi_m\rangle \otimes |\chi_\sigma\rangle = e^{i\hat{S}}|\psi_{m,\sigma}\rangle$, where $|\phi_m\rangle$ is a bus-only eigenstate, $|\chi_\sigma\rangle$ a probe state, and $|\psi_{m,\sigma}\rangle$ an eigenstate for finite α. Under this transformation, the Hamiltonian must separate into a bus term and a probe term, since the corresponding eigenstates are product states, $\mathcal{H}_S = e^{i\hat{S}}\left(\mathcal{H}_b + \mathcal{H}_{p-b}\right) e^{-i\hat{S}} = \mathcal{H}_p + \mathcal{H}_b^{'}$; the construction of this canonical transformation is generally achieved in a perturbation expansion in α [19], but we choose to keep it unspecified for the moment. If we use the canonical transformation in the expressions of thermal averages, we can easily rewrite them in terms of $\mathcal{H}_\mathcal{S}$; on the other hand, the assumption of a robust gap, *i.e.,* the lowest lying states of the full system, which map to the product of $|\phi_0\rangle$ and the probe singlet or triplet, are well separated from remaining states by a gap $\Delta(\alpha) \gg k_B T$, allows the neglect of thermal occupation of states which map to excited states of the bus; one obtains

$$\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b \rangle = \frac{\mathrm{Tr}_p\left[e^{-\beta\mathcal{H}_p}\sum_m A_m \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b A_m^\dagger\right]}{\mathrm{Tr}_p\left[e^{-\beta\mathcal{H}_p}\right]},$$

where $\mathrm{Tr}_p(\dots)$ is a trace over probe states, and $A_m = \langle\phi_0|e^{i\hat{S}}|\phi_m\rangle$ is a probe-only operator. Rotational symmetry implies that $\sum_m A_m \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b A_m^\dagger$ must be a scalar operator [6]; therefore, $\sum_m A_m \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b A_m^\dagger = \eta + (1 - \Phi)\, \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b$, where, by construction, η and Φ are temperature independent. This obviously entails $\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle = \eta + (1-\Phi)\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle_{\mathrm{can}}$, where $\langle \dots \rangle_{\mathrm{can}}$ is an average with the Hamiltonian $\mathcal{H}_p$, which has the form $\mathcal{H} = \frac{1}{4}\mathcal{J}\boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b$, implied by symmetry. By expressing $\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle$ in terms of J_{ab}, using Eq.(2), and $\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle_{\mathrm{can}}$ in terms of $\mathcal{J}$, one easily derives Eq. (3).

The actual calculation of these parameters, $\mathcal{J}$, Φ and η, can only be done in perturbation theory, following the approach of Schrieffer and Wolff [19]. The calculation of the effective coupling $\mathcal{J}$ has been discussed in [7]; to calculate the canonical corrections η and Φ we start from

$$\begin{aligned}\langle\phi_0|e^{i\hat{S}}\boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b e^{-i\hat{S}}|\phi_0\rangle \;&=\; \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b + i\langle\phi_0|\left[\hat{S}, \tau_a \cdot \tau_b\right]|\phi_0\rangle \\ &-\; \frac{1}{2}\langle\phi_0|\left[\hat{S}, \left[\hat{S}, \tau_a \cdot \tau_b\right]\right]|\phi_0\rangle + \mathcal{O}(\alpha^3)\end{aligned}$$

and use the generator prescribed by $\mathcal{H}_{p-b} + \left[i\hat{S}, \mathcal{H}_b\right] = 0$ [19], to obtain

$$\Phi \;=\; 4\alpha^2 J^2 \sum_{m>0}\left(\frac{1}{(E_m - E_0)}|\langle\phi_0|\left(S_A^z - S_B^z\right)|\phi_m\rangle|\right)^2 \quad (5)$$

$$\eta \;=\; 0 + \mathcal{O}(\alpha^4). \quad (6)$$

The fact that η is of higher order than Φ means that, for weak coupling, we have a simpler result than would be implied by rotational symmetry alone, namely, $\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle = (1-\Phi)\langle \boldsymbol{\tau}_a \cdot \boldsymbol{\tau}_b\rangle_{can}$, and J_{ab} given by Eq.(3) with $\eta = 0$. In fact, for $\alpha \leq 0.1$, a careful inspection shows that the fits we present are virtually indistinguishable from the fits with $\eta = 0$.

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